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ABSTRACT

Fluid flow, temperature prediction, thermal response and light-off behavior of the catalytic converter were investigated using Computational Fluid Dynamics (CFD), combined with a conjugate heat transfer and a chemical reaction model. There are two objectives in this study: one to predict the maximum operation temperature for appropriate materials selection; and the other, to develop a numerical model which can be adjusted to reflect changes in the catalyst/washcoat formulation to accurately predict effects on the flow, temperature and light-off behavior.

Temperature distributions were calculated for exhaust gas, catalyzed substrate, mounting mat and converter skin. Converter shell skin temperature was obtained for different mat materials. By changing reactant mass concentrations and noble metal loading, the converter light-off behavior, thermal response and temperature distributions were changed.

INTRODUCTION

In converter designs used on gasoline engines, there are two major concerns; the converter performance as it related to emissions, and the high temperature durability.

It is well known that the converter performance is substantially affected by the flow distribution within the substrate. A uniform flow distribution increases the conversion efficiency, causes less pressure drop and increases engine performance. Flow distribution in a converter assembly is controlled by the geometry configurations of inlet and outlet cones, the substrate and the exhaust gas compositions. Optimized geometry designs based on uniform flow distribution are crucial to a converter performance. The effects of poor flow distribution on converter performance and durability have been studied by many researchers [1].

Considering the high temperature durability, the most important issue is to accurately predict the maximum operating temperature of the shell, mat and substrate. This temperature prediction then defines the material selections for the mat, shell and cones, and allows an assessment to be made as to the necessity of heat shielding. The high skin temperature of the converter results from the high inlet gas temperature, and the heat released from the chemical reactions which take place on the substrate surface. Chemical reactions also change the thermal and species fields, which in turn affect the flow field. So, considerations of chemical reactions in the converter development process are also crucial.

Another issue in the converter development is the converter light-off behavior. Up to 80% of all HC emissions during the FTP test cycle occurs in the first 100 ~ 150 seconds following the engine start. Therefor, the length of time which the converter takes to reach the catalyst light-off temperature is of particular interest. The light-off study gives the temperature evolution and the conversion efficiency. Understanding the light-off behavior is important in order to develop high performance converters.

Converter thermal and conversion characteristics have been studied by many researchers. Most of previous modeling studies assumed adiabatic thermal boundary conditions and a uniform flow in substrates for converters. Thus, only one substrate channel was modeled [2]. Chen et al. [3] performed three-dimensional studies, but only thermal field was solved and the flow was measured. Jeong and Kim [4] modeled 3D thermal reactive fluid flow in converters, their work focused on geometry effects on thermal behaviors.

In actual converters, the flow is known to be three-dimensional turbulent. Flow field and thermal field are closely coupled in the light-off period and the flow is compressible. Chemical reactions on the substrate surface create heat sources for the thermal field. In order to study thermal and conversion characteristics of converters, the numerical model must handle flow, thermal and chemical reactions together. With the advance of high performance computers and accurate numerical schemes, Computational Fluid Dynamics (CFD) can be used to simulate the complex flow physics inside the converter. It can provide complete, fast and accurate analysis of the thermal fluid flow, cut testing costs and reduce design circles. In converter designs, CFD is used to analyze flow distribution,

pressure drop, temperature profile and chemical reactions. It performs both static and transient analysis. The transient analysis is necessary for the light-off study.

In this paper, (CFD) was used to simulate the three-dimensional turbulent compressible thermal fluid flow with chemical reactions on the substrate surfaces. The first objective of this paper was to predict temperature and select the appropriate materials for converters. The second objective was to develop a numerical model which can be adjusted based on the catalyst coating (provided by the coater), so the model can predict the flow, temperature, light-off behavior and conversion characteristics properly and accurately.

The geometry and operating conditions are described in the next section. Then the analysis approach, results and discussions are presented. Conclusions were drawn in the last section.

GEOMETRY AND OPERATING CONDITIONS

The geometry of the converter design examined in this paper is shown in Figure 1. A 3.15"x4.75"x5.49" ceramic substrate with 400/4 mil cell density is placed in this system. A 8.2 mm gap exists between the substrate and shell, and this gap is filled with a layer of mat. Two different mats were used: 3M Interam 100 and Saffil. Both the inlet and outlet cones are dual wall designs with Saffil filled between the two walls. The shell is 409 stainless steel with 1.4 mm thickness.

The inlet exhaust gas flow rate is held constant at 7.81 lb/min. Three species (CO, O_2, C_3H_6) are considered in the chemical reaction model which simulates a Platinum (Pt) catalyst converter. The inlet species mass fractions are also held constant, and two concentrations were used (Table 1).

Table 1. Inlet Species Concentrations (Mass Fraction)

	Concentration 1	Concentration 2
CO	0.0346	0.0048
C3H6	0.001335	0.00065
O2	0.085	0.002

Two noble metal loadings were used: $2.5x10^5$ m^2/m^3 (catalyst surface area per unit reactor volume) which represents fresh commercial converters; $3.0x10^4$ m^2/m^3 which represents typical in-use converters. The inlet temperature increases from 20°C (ambient temperature) to 1050°C in the first 30 seconds in the transient analysis and is held constant at 1050°C in the static analysis.

Properties of materials used in this study are listed in table 2.

Table 2. Material Properties

	Density (kg/m^3)	Specific heat (J/kg.K)	Thermal conductivity (W/m.K)
Air	Ideal law	1159	.0715
Substrate	2510	1110	.25
Interam 100	993	1110	.194
Saffil	330	1110	.13
Steel	7800	724	27.2

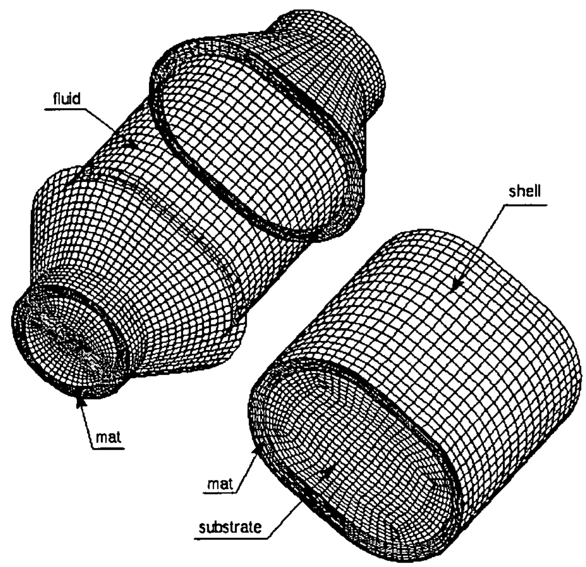


Figure 1. Geometry

ANALYSIS APPROACH

FLUID FLOW – Three-dimensional compressible turbulent flow was solved. The governing equations are Navier-Stockes equations which can be found in most common fluid dynamics books. The κ-ε turbulence model was used. Ideal gas law was used to count for the compressibility of the gas.

A porous media model was used to treat the substrate in the flow analysis. This porous media model simulates a pressure resistant to the fluid [5]. The flow within the substrate channels is assumed to be a fully developed laminar flow. The parameters used in this porous media model were calculated based on the substrate properties: the material, cell density, wall thickness and coating.

To predict the flow distribution, the most important parameter is flow uniformity. Flow uniformity can be defined in several ways. In this study, flow uniformity is defined as the ratio of the high velocity area to the total frontal area of a substrate. The high velocity is defined as a percentage (65%) of the maximum velocity in this frontal section of the substrate.

HEAT TRANSFER – A conjugate heat transfer model was used for the thermal analysis, which simulates heat transfer in gas, convection between the exhaust gas and mat, the conduction in the mat and shell, the convection and radiation between the shell and ambient air, and the heat transfer between the gas and substrate. The energy equations for gas and solids can be found in most common heat transfer books.

In the gas energy equation, there is a source term which counts for the heat transfer between the exhaust gas and substrate. In the heat conduction equation for the substrate, there are two source terms: one for heat transfer between exhaust gas and the substrate, one for the heat released from chemical reactions. The heat transfer coefficient between the gas and substrate is calculated based on a constant Nusselt number (Nu=3.66) for fully developed laminar channel flow. The heat transfer between the converter shell and surrounding air is free convection and radiation, which were considered through a comprehensive heat transfer coefficient. The conduction in the substrate was considered to be anisotropic.

CHEMICAL REACTION AND MASS TRANSFER – In this study, a platinum catalyst converter was simulated. The oxidation reactions of CO and hydrocarbons were considered. The hydrocarbons were represented by propylene which is the easily oxidized hydrocarbon (the easily oxidized hydrocarbons constitute about 80% of the total hydrocarbons found in a typical exhaust gas [6]). The chemical reactions modeled are:

$$2CO+O_2 \rightarrow 2CO_2$$
$$2C_3H_6+9O2 \rightarrow 6CO_2+6H_2O$$

A surface reaction model was used for the chemical reaction analysis, which simulates reactions taking place on the substrate surface and the heat released from the reactions. The kinetic model proposed by Voltz et al. was used [6]. The reaction rates are temperature dependent and of Langmuir-Hinshewood type expressions.

Standard mass transport equations were solved for gas phase species CO, C_3H_6 and O_2 in exhaust gas. These equations can be found in most common transport phenomena books. There is a source term in each of these three mass transport equations. This source term accounts for the mass transfer between the gas phase species in the exhaust gas flow and the solid phase species on the substrate surface. The mass transfer coefficient between the gas and the substrate surface was calculated using a constant Sherwood (Sh) number for fully developed laminar flow. The last equation in this model is a conservation equation which takes into account the mass balance for these three species in the gas and solid phases.

NUMERICAL METHODS – The computational mesh consists of 80K cells, which includes the fluid, substrate, mat and the shell. The mesh was generated using ICEMCFD. Star-CD was incorporated with all theoretical models to do the analysis.

In this study, the three-dimensional compressible turbulent flow was analyzed with the heat transfer and chemical reactions for both the static and transient simulations.

RESULTS AND DISCUSSIONS

Numerical results were obtained for flow distribution, pressure drop, temperature profiles, temperature evolution in light-off period, and the conversion efficiency of CO and C_3H_6.

In this study, the major focus was on temperature prediction and conversion characteristics, so a relatively simple geometry was chosen. In this geometry, both inlet and outlet cones are straight and a good flow is expected. It is found from the computations that the flow is very uniform in the substrate and the uniformity is 99%. The ratio of the maximum velocity to the minimum velocity is only 1.15 inside the substrate. The total pressure drop of this converter is about 5 KPa, of which 88% is from the substrate, 7% from the inlet cone and 5% from the outlet cone.

Figure 2 (a)--(e) are the temperature distributions in a section which is cutting through the center of the converter along the longer axis. The higher concentrations were used (concentration 1, in Table 1) and the mat material is Interam 100. Results at 30, 60, 90 and 120 seconds after the engine start, simulates the light-off period. The substrate thermal response to the inlet heat and also to the chemical reactions can be seen clearly. The temperature of the skin, mat, substrate and the fluid can be obtained at any points. The insulation effects of the mat can be seen clearly. When steady state is reached, the highest substrate temperature is 1393°C; the lowest skin temperature is 308°C. The substrate reaches the highest temperature and becomes stable in about 3 minutes. It takes about 20 minutes for the skin to reach the steady temperature.

Figure 2 is the temperature vs. longer radius at the center frontal surface of the substrate for two different mats: Interam 100 and Saffil. The higher concentrations (concentration1 , Table 1) were used. It can be seen that different skin temperature is obtained for different mats. The skin temperature difference is about 100°C along the longer radius. Saffil gives lower skin temperature because of its lower thermal conductivity.

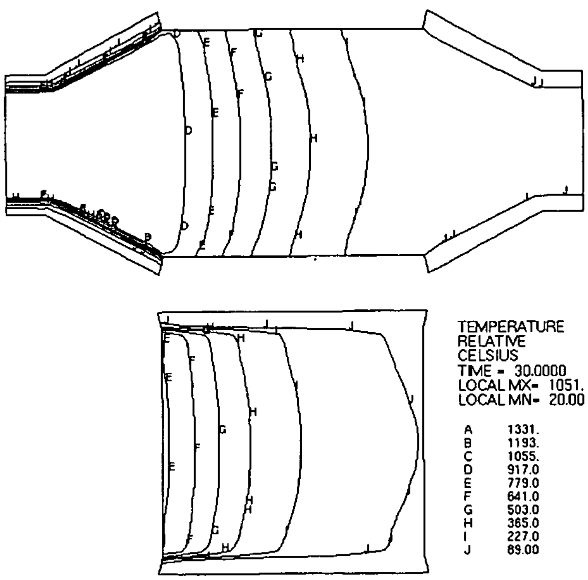
Figure 4 is the conversion efficiencies at two different concentrations for the light-off period. It can be seen that, for lower concentrations, the converter has slightly earlier light-off and higher conversion efficiencies when conversion becomes stable. The plot also shows that the converter becomes effective in about 20 seconds after the engine start. After 45 seconds, the conversion efficiency reaches its maximum value and becomes stable.

Figure 5 is the thermal response of the converter. Temperature vs. time is plotted for three points on the center axis of the substrate: front, middle and rear. Two concentrations were used (Table 1). It can be seen that the rate

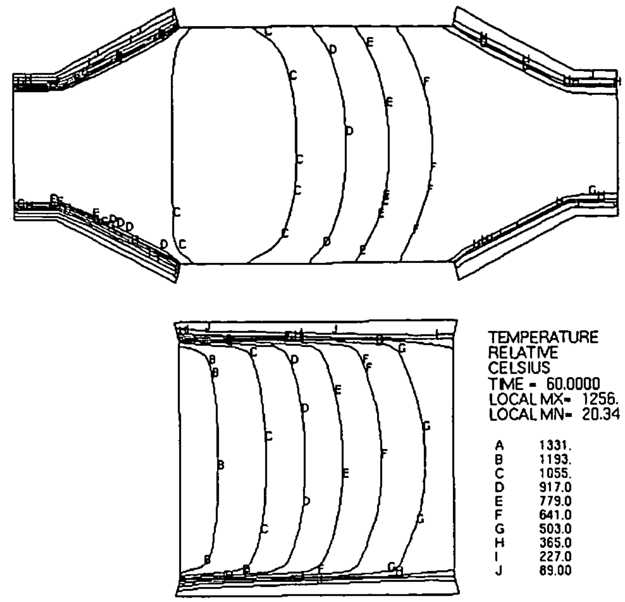
of temperature increase at front point is much higher than that for the other two points. With higher concentrations, the temperature increasing rate is higher and the substrate reaches a higher stable temperature.

Figure 6 is the temperature vs. the longer radius at the center frontal surface of the substrate for two different concentrations (Table 1) at steady state. It can be seen that the temperature of substrate and skin is higher for higher concentrations. The temperature difference is about 285°C on the substrate for these two concentrations.

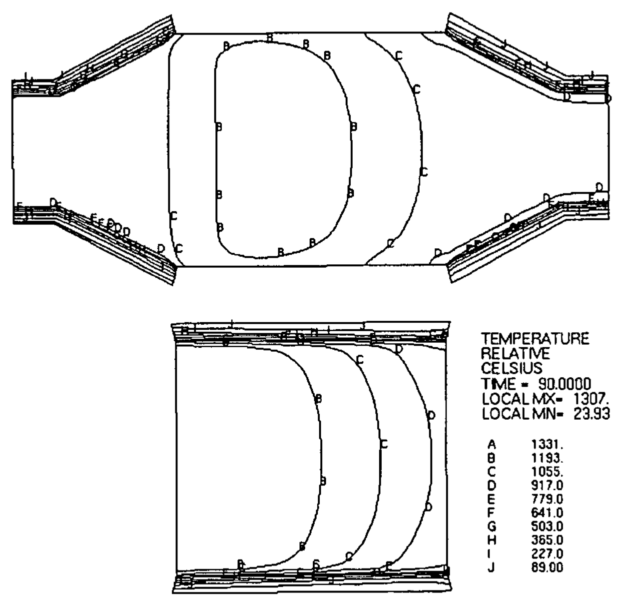
Figure 7 is the conversion efficiency for different noble metal loading. Concentration 1 in Table 1 was used. The higher loading (2.5×10^5 m^2/m^3 catalyst surface area per unit reactor volume) represents fresh commercial converters; the lower loading (3.0×10^4 m^2/m^3) represents typical in-use converters. It can be seen that the converter has earlier light-off for the higher catalyst loading. After the conversion becomes stable, the efficiency is the same for both catalyst loadings.



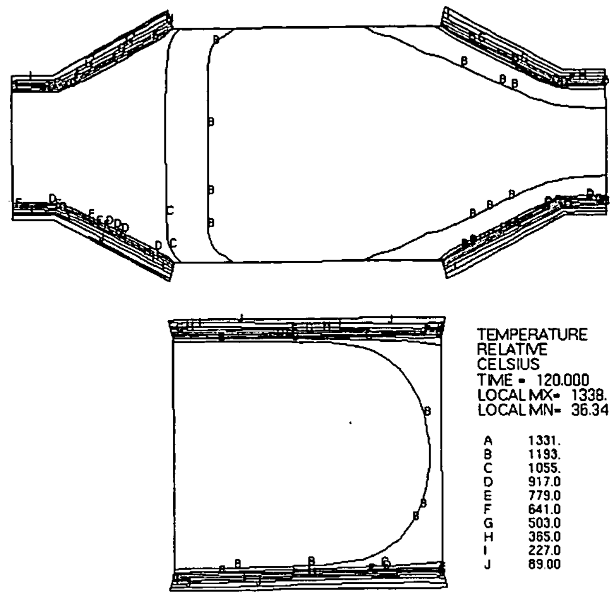
(a) 30 sec



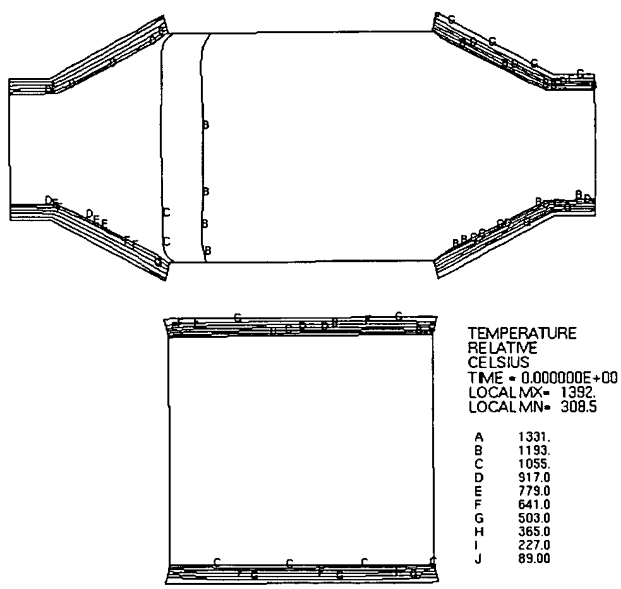
(b) 60 sec



(c) 90 sec



(d) 120 sec



(e) steady state

Figure 2. Temperature evolution for Interam 100
$CO=.0346$ $C_3H_6=.001335$ $O_2=.085$

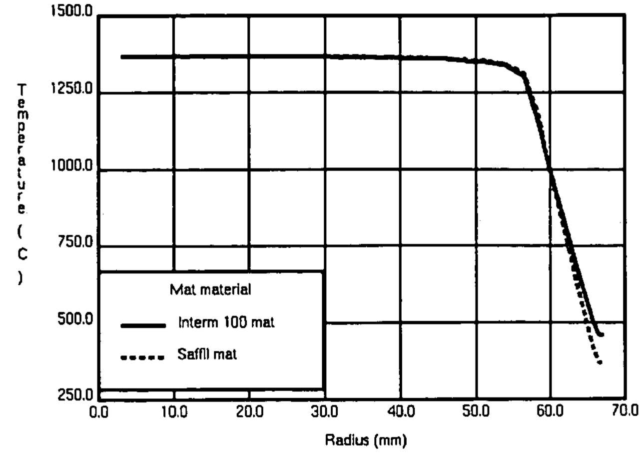


Figure 3. Temperature vs. radius for different mats at steady state
$CO=.0346$ $C_3H_6=.001335$ $O_2=.085$

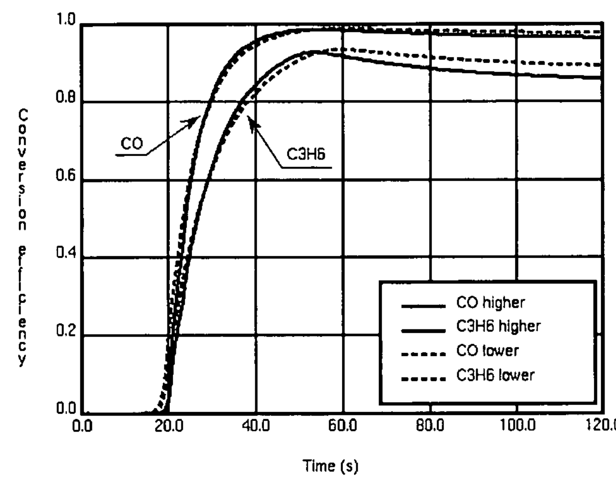


Figure 4. Conversion efficiency at different concentrations

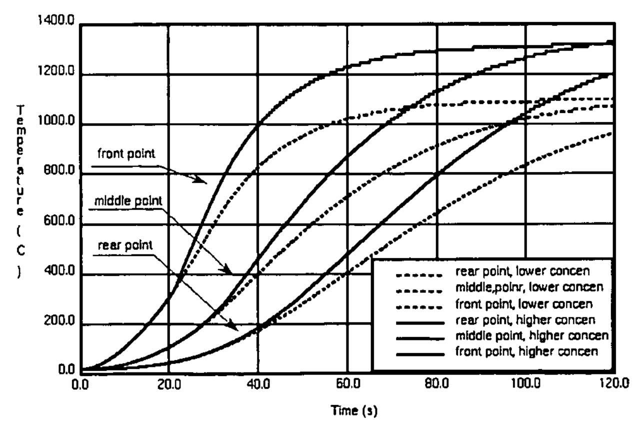


Figure 5. Thermal response at three points for two concentrations

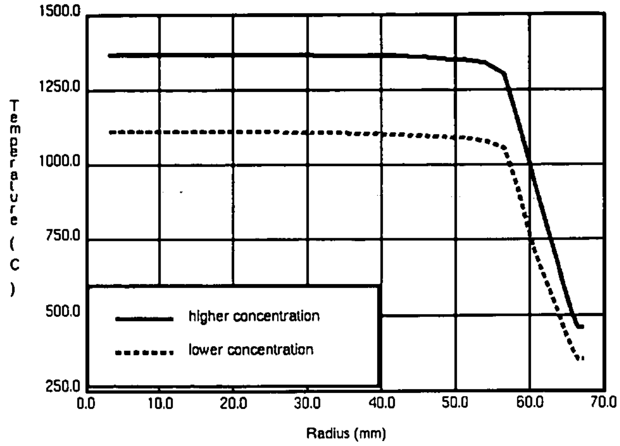


Figure 6. Temperature vs. radius for different concentrations at steady state Interam 100 mat

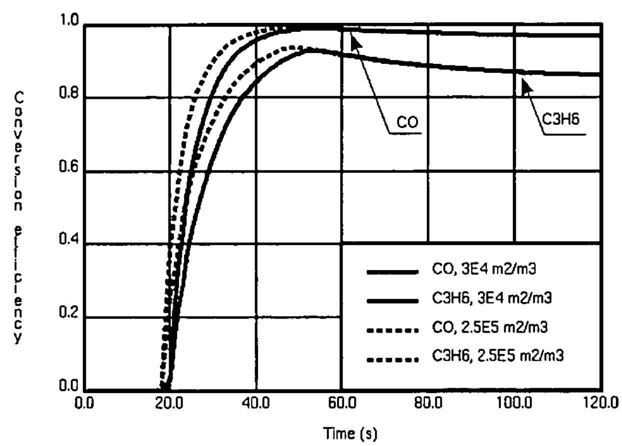


Figure 7. Conversion efficiency for different noble metal loading
CO=.0346 C_3H_6=.001335 O_2=.085

CONCLUSION

This study investigated the flow characteristics, the temperature distribution and thermal response, the light-off behavior and conversion efficiency of a converter. From above analysis, the following conclusions can been drawn.

1. The temperature of the fluid, catalyzed substrate, mat and skin of the converter can be predicted in three-dimensional for both steady state and light-off period.
2. By changing the concentrations, the converter thermal response, conversion characteristics and steady state temperature can be changed.
3. By changing the noble metal loadings, the conversion characteristics of the converter can be changed.
4. Based on catalyst coating provided by coaters, this numerical model can used adjusted to have the corresponding thermal response and conversion characteristics, and to predict temperature accurately.
5. Correlation work with all these variables is needed to validate the numerical predictions with experimental results.

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